



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:39 AM EDT

PDB ID : 8DSN / pdb\_00008dsn  
Title : Peptidylglycine alpha hydroxylating monooxygenase, Q272A  
Authors : Arias, R.J.; Blackburn, N.J.  
Deposited on : 2022-07-22  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

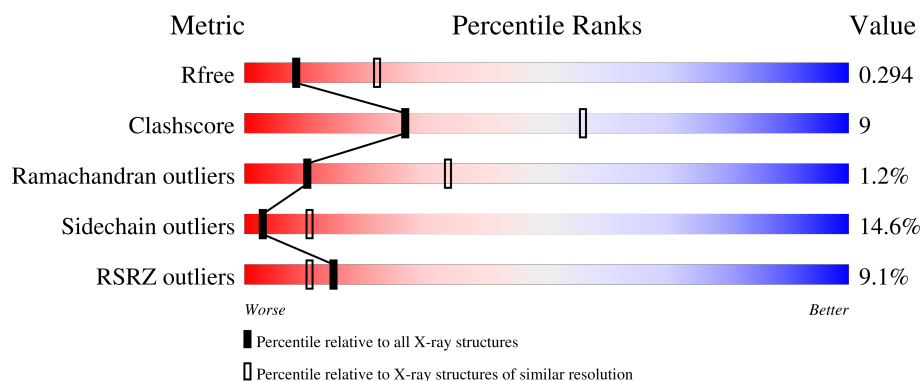
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	<div> <div>9%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	K	310	<div> <div>9%</div> <div>68%</div> <div>24%</div> <div>5% • •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidylglycine alpha-amidating monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2396	1527	403	440	26			
1	K	305	Total	C	N	O	S	0	0	0
			2374	1515	397	436	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	GLN	engineered mutation	UNP P14925
K	272	ALA	GLN	engineered mutation	UNP P14925

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cu	0	0
			3	3		
2	K	3	Total	Cu	0	0
			3	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		

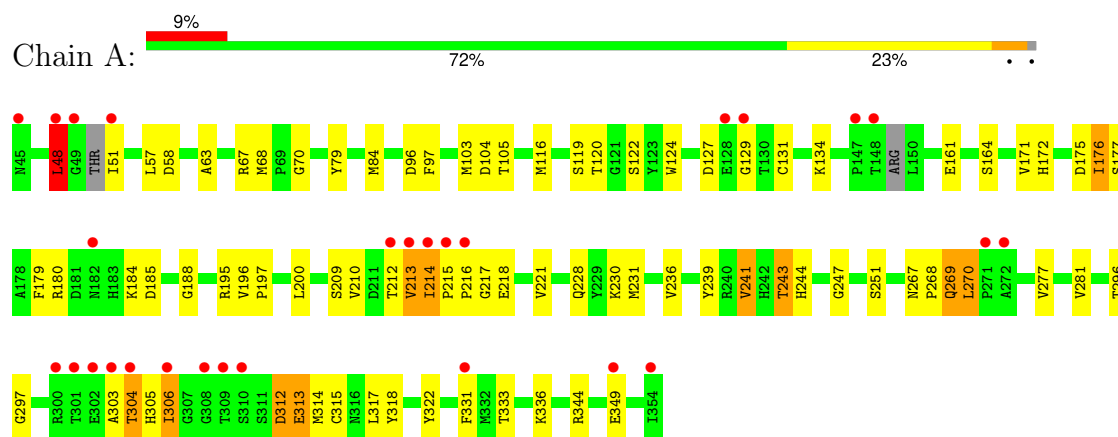
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	K	13	Total	O	0	0
			13	13		

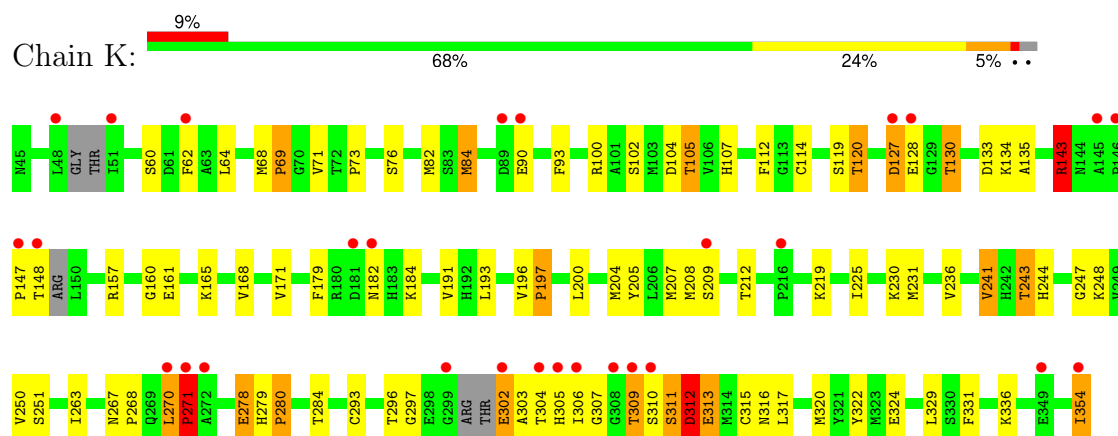
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Peptidylglycine alpha-amidating monooxygenase



- Molecule 1: Peptidylglycine alpha-amidating monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.88Å 53.49Å 86.06Å 84.71° 89.82° 77.96°	Depositor
Resolution (Å)	38.05 – 2.80 38.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.05-2.80) 98.9 (38.05-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.75 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.198 , 0.296 0.208 , 0.294	Depositor DCC
$R_{free}$ test set	835 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.03	0/2462	1.29	6/3346 (0.2%)
1	K	1.01	1/2439 (0.0%)	1.33	6/3314 (0.2%)
All	All	1.02	1/4901 (0.0%)	1.31	12/6660 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	197	PRO	C-O	-7.19	1.15	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	127	ASP	N-CA-C	-8.35	102.36	112.54
1	A	127	ASP	N-CA-C	-6.09	105.60	113.16
1	K	69	PRO	N-CA-CB	-5.66	99.02	102.81
1	A	103	MET	CA-C-N	5.45	127.86	120.44
1	A	103	MET	C-N-CA	5.45	127.86	120.44
1	K	120	THR	CA-C-N	-5.35	116.79	122.30
1	K	120	THR	C-N-CA	-5.35	116.79	122.30
1	A	180	ARG	N-CA-C	-5.34	105.35	111.07
1	K	311	SER	N-CA-C	-5.25	105.61	112.23
1	A	269	GLN	N-CA-C	-5.21	105.80	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	157	ARG	CB-CA-C	5.12	118.19	109.84
1	A	188	GLY	CA-C-O	-5.01	117.45	120.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	104	ASP	Peptide
1	K	244	HIS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2396	0	2312	44	0
1	K	2374	0	2288	45	0
2	A	3	0	0	0	0
2	K	3	0	0	0	0
3	A	24	0	32	2	0
3	K	12	0	16	2	0
4	A	15	0	0	5	0
4	K	13	0	0	0	0
All	All	4840	0	4648	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:HIS:HA	4:A:502:HOH:O	1.73	0.88
1:A:243:THR:HG21	1:A:247:GLY:HA3	1.59	0.84
1:A:48:LEU:H	1:A:48:LEU:HD13	1.47	0.80
1:A:68:MET:HE3	1:A:171:VAL:HG23	1.65	0.77
1:A:214:ILE:HG23	1:A:221:VAL:HG21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:GLY:O	1:K:165:LYS:NZ	2.24	0.70
1:A:267:ASN:HB3	1:A:270:LEU:HD22	1.76	0.67
1:A:200:LEU:HD13	1:A:322:TYR:CE1	2.31	0.66
1:K:278:GLU:H	1:K:278:GLU:CD	2.05	0.65
1:K:130:THR:HG23	1:K:168:VAL:HG11	1.79	0.65
1:K:68:MET:HE3	1:K:171:VAL:HG23	1.79	0.64
1:A:244:HIS:HB2	1:A:313:GLU:CD	2.25	0.62
1:A:213:VAL:HG22	4:A:502:HOH:O	2.01	0.61
1:K:102:SER:HB2	1:K:105:THR:HG22	1.83	0.60
1:K:243:THR:HG22	1:K:268:PRO:HB2	1.82	0.60
1:K:212:THR:HB	1:K:306:ILE:HG12	1.84	0.60
1:A:244:HIS:O	1:A:269:GLN:NE2	2.36	0.58
1:K:205:TYR:OH	3:K:405:GOL:O2	2.22	0.58
1:K:205:TYR:HH	3:K:405:GOL:HO2	1.51	0.57
1:A:239:TYR:HA	1:A:318:TYR:O	2.05	0.56
1:K:107:HIS:HA	1:K:143:ARG:HD3	1.86	0.56
1:K:209:SER:OG	1:K:315:CYS:HB3	2.07	0.55
1:K:296:THR:HG22	1:K:297:GLY:H	1.72	0.55
1:K:309:THR:HG22	1:K:311:SER:H	1.72	0.55
1:K:212:THR:HB	1:K:306:ILE:CG1	2.38	0.54
1:A:68:MET:HE3	1:A:171:VAL:CG2	2.36	0.54
1:K:309:THR:O	1:K:312:ASP:N	2.41	0.54
1:K:93:PHE:CE1	1:K:197:PRO:HA	2.43	0.52
1:A:212:THR:OG1	1:A:306:ILE:HD11	2.10	0.51
1:K:207:MET:HE2	1:K:225:ILE:HG22	1.93	0.51
1:K:243:THR:HG21	1:K:247:GLY:HA3	1.92	0.50
1:K:68:MET:HE3	1:K:171:VAL:CG2	2.42	0.49
1:K:200:LEU:HD13	1:K:322:TYR:CE1	2.47	0.49
1:A:216:PRO:C	4:A:505:HOH:O	2.56	0.49
1:A:244:HIS:CE1	1:A:314:MET:SD	3.06	0.49
1:A:129:GLY:O	1:A:131:CYS:N	2.42	0.49
1:A:243:THR:HG22	1:A:268:PRO:HB2	1.96	0.48
1:A:243:THR:HG23	1:A:244:HIS:O	2.14	0.48
1:A:244:HIS:HB2	1:A:313:GLU:OE2	2.13	0.48
1:K:208:MET:HA	1:K:315:CYS:O	2.14	0.48
1:A:236:VAL:HG12	1:A:277:VAL:HG21	1.96	0.47
1:A:196:VAL:O	1:A:197:PRO:C	2.56	0.47
1:A:312:ASP:N	1:A:312:ASP:OD1	2.47	0.47
1:A:79:TYR:CE1	1:A:172:HIS:CD2	3.02	0.47
1:K:309:THR:HB	1:K:312:ASP:OD2	2.14	0.47
1:A:200:LEU:HD13	1:A:322:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:HB3	1:A:124:TRP:CD2	2.50	0.46
1:K:191:VAL:HG12	1:K:193:LEU:HD22	1.98	0.46
1:K:241:VAL:HB	1:K:250:VAL:HG11	1.98	0.46
1:A:213:VAL:HA	1:A:304:THR:O	2.16	0.46
1:K:73:PRO:HD2	1:K:179:PHE:CE1	2.51	0.46
1:A:231:MET:HG2	3:A:407:GOL:H11	1.97	0.46
1:K:112:PHE:CD1	1:K:130:THR:HG21	2.51	0.46
1:K:204:MET:HE1	1:K:320:MET:HG3	1.98	0.45
1:A:214:ILE:O	1:A:303:ALA:HA	2.16	0.45
1:A:217:GLY:N	4:A:505:HOH:O	2.49	0.45
1:K:302:GLU:HB3	1:K:303:ALA:H	1.51	0.45
1:A:96:ASP:OD1	1:A:97:PHE:N	2.50	0.44
1:K:112:PHE:CD2	1:K:135:ALA:HB1	2.52	0.44
1:K:307:GLY:N	1:K:313:GLU:O	2.50	0.44
1:A:215:PRO:C	4:A:505:HOH:O	2.61	0.44
1:K:267:ASN:HB2	1:K:354:ILE:HG23	2.00	0.44
1:A:241:VAL:HG12	1:A:317:LEU:HD13	2.00	0.43
1:K:241:VAL:HG12	1:K:317:LEU:HD12	2.01	0.43
1:A:119:SER:OG	1:A:120:THR:N	2.52	0.43
1:A:241:VAL:HG12	1:A:317:LEU:CD1	2.48	0.43
1:K:107:HIS:HD2	1:K:143:ARG:CZ	2.32	0.43
1:K:208:MET:HB3	1:K:316:ASN:HD22	1.83	0.43
1:A:84:MET:HE2	1:A:84:MET:HB3	1.88	0.43
1:A:57:LEU:HD11	1:A:63:ALA:HB2	2.00	0.42
1:K:60:SER:HB2	1:K:196:VAL:HG23	2.01	0.42
1:K:69:PRO:HD2	1:K:71:VAL:HG13	2.01	0.42
1:K:250:VAL:HG22	1:K:293:CYS:SG	2.59	0.42
1:K:236:VAL:HG11	1:K:263:ILE:HG23	2.01	0.42
1:K:279:HIS:O	1:K:280:PRO:C	2.63	0.42
1:A:179:PHE:HZ	1:A:185:ASP:HB2	1.85	0.42
1:A:231:MET:HG2	3:A:407:GOL:C1	2.50	0.41
1:K:114:CYS:HB2	1:K:133:ASP:OD1	2.20	0.41
1:A:196:VAL:HG13	1:K:231:MET:HA	2.02	0.41
1:K:270:LEU:O	1:K:271:PRO:C	2.63	0.41
1:A:48:LEU:H	1:A:48:LEU:CD1	2.18	0.41
1:A:218:GLU:O	1:A:297:GLY:N	2.52	0.41
1:A:243:THR:HG23	1:A:244:HIS:N	2.34	0.40
1:A:305:HIS:O	1:A:313:GLU:N	2.48	0.40
1:K:243:THR:HG22	1:K:268:PRO:CB	2.48	0.40
1:K:119:SER:OG	1:K:120:THR:N	2.55	0.40
1:A:176:ILE:H	1:A:176:ILE:HG13	1.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:64:LEU:HG	1:K:84:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/310 (97%)	279 (92%)	20 (7%)	3 (1%)	12	38
1	K	297/310 (96%)	271 (91%)	22 (7%)	4 (1%)	9	31
All	All	599/620 (97%)	550 (92%)	42 (7%)	7 (1%)	10	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	58	ASP
1	A	70	GLY
1	K	147	PRO
1	K	271	PRO
1	K	143	ARG
1	K	312	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/264 (99%)	225 (86%)	37 (14%)	3	12
1	K	260/264 (98%)	221 (85%)	39 (15%)	3	10
All	All	522/528 (99%)	446 (85%)	76 (15%)	3	11

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	51	ILE
1	A	67	ARG
1	A	104	ASP
1	A	105	THR
1	A	116	MET
1	A	122	SER
1	A	134	LYS
1	A	161	GLU
1	A	164	SER
1	A	175	ASP
1	A	176	ILE
1	A	177	SER
1	A	184	LYS
1	A	195	ARG
1	A	209	SER
1	A	210	VAL
1	A	213	VAL
1	A	214	ILE
1	A	228	GLN
1	A	230	LYS
1	A	241	VAL
1	A	243	THR
1	A	251	SER
1	A	270	LEU
1	A	281	VAL
1	A	296	THR
1	A	304	THR
1	A	306	ILE
1	A	312	ASP
1	A	313	GLU
1	A	315	CYS
1	A	331	PHE
1	A	333	THR
1	A	336	LYS

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	349	GLU
1	K	62	PHE
1	K	76	SER
1	K	82	MET
1	K	84	MET
1	K	90	GLU
1	K	100	ARG
1	K	105	THR
1	K	127	ASP
1	K	128	GLU
1	K	130	THR
1	K	134	LYS
1	K	143	ARG
1	K	148	THR
1	K	161	GLU
1	K	182	ASN
1	K	184	LYS
1	K	219	LYS
1	K	230	LYS
1	K	241	VAL
1	K	243	THR
1	K	248	LYS
1	K	251	SER
1	K	270	LEU
1	K	271	PRO
1	K	278	GLU
1	K	280	PRO
1	K	284	THR
1	K	302	GLU
1	K	304	THR
1	K	305	HIS
1	K	309	THR
1	K	310	SER
1	K	312	ASP
1	K	313	GLU
1	K	324	GLU
1	K	329	LEU
1	K	331	PHE
1	K	336	LYS
1	K	354	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	183	HIS
1	A	235	HIS
1	A	279	HIS
1	A	316	ASN
1	K	235	HIS
1	K	316	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	K	404	-	5,5,5	0.18	0	5,5,5	0.50	0
3	GOL	A	404	-	5,5,5	0.13	0	5,5,5	0.27	0
3	GOL	K	405	-	5,5,5	0.16	0	5,5,5	0.36	0
3	GOL	A	407	-	5,5,5	0.11	0	5,5,5	0.28	0
3	GOL	A	405	-	5,5,5	0.17	0	5,5,5	0.39	0
3	GOL	A	406	-	5,5,5	0.21	0	5,5,5	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	K	404	-	-	3/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	K	405	-	-	2/4/4/4	-
3	GOL	A	407	-	-	4/4/4/4	-
3	GOL	A	405	-	-	4/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3
3	K	404	GOL	O1-C1-C2-C3
3	K	405	GOL	O1-C1-C2-O2
3	K	405	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-C3
3	A	406	GOL	O1-C1-C2-C3
3	A	407	GOL	O1-C1-C2-C3
3	A	407	GOL	C1-C2-C3-O3
3	K	404	GOL	C1-C2-C3-O3
3	K	404	GOL	O1-C1-C2-O2
3	A	406	GOL	O1-C1-C2-O2
3	A	405	GOL	O2-C2-C3-O3
3	A	407	GOL	O1-C1-C2-O2
3	A	405	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2
3	A	407	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	405	GOL	2	0
3	A	407	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	308/310 (99%)	0.46	28 (9%) 15 11	13, 36, 123, 169	0
1	K	305/310 (98%)	0.47	28 (9%) 14 10	15, 38, 112, 151	0
All	All	613/620 (98%)	0.47	56 (9%) 15 11	13, 37, 119, 169	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	148	THR	6.7
1	A	212	THR	5.9
1	A	213	VAL	5.3
1	K	51	ILE	5.1
1	A	148	THR	4.7
1	A	304	THR	4.6
1	K	48	LEU	4.5
1	A	354	ILE	4.4
1	A	300	ARG	4.1
1	A	303	ALA	3.9
1	K	147	PRO	3.8
1	A	309	THR	3.8
1	A	310	SER	3.6
1	A	49	GLY	3.5
1	A	271	PRO	3.5
1	A	51	ILE	3.5
1	A	129	GLY	3.4
1	K	128	GLU	3.4
1	K	310	SER	3.4
1	A	214	ILE	3.4
1	K	308	GLY	3.3
1	A	45	ASN	3.2
1	K	145	ALA	3.2
1	A	215	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	2.9
1	K	354	ILE	2.8
1	K	309	THR	2.8
1	A	301	THR	2.8
1	A	216	PRO	2.8
1	A	308	GLY	2.8
1	K	146	PRO	2.7
1	K	271	PRO	2.7
1	A	128	GLU	2.6
1	A	331	PHE	2.6
1	K	299	GLY	2.6
1	K	306	ILE	2.6
1	A	272	ALA	2.6
1	K	127	ASP	2.6
1	K	216	PRO	2.5
1	A	306	ILE	2.5
1	K	305	HIS	2.5
1	K	89	ASP	2.4
1	K	304	THR	2.4
1	A	147	PRO	2.4
1	K	349	GLU	2.3
1	K	90	GLU	2.3
1	A	302	GLU	2.3
1	K	181	ASP	2.3
1	K	270	LEU	2.2
1	K	302	GLU	2.2
1	K	182	ASN	2.1
1	A	182	ASN	2.1
1	K	62	PHE	2.1
1	K	272	ALA	2.0
1	K	209	SER	2.0
1	A	349	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

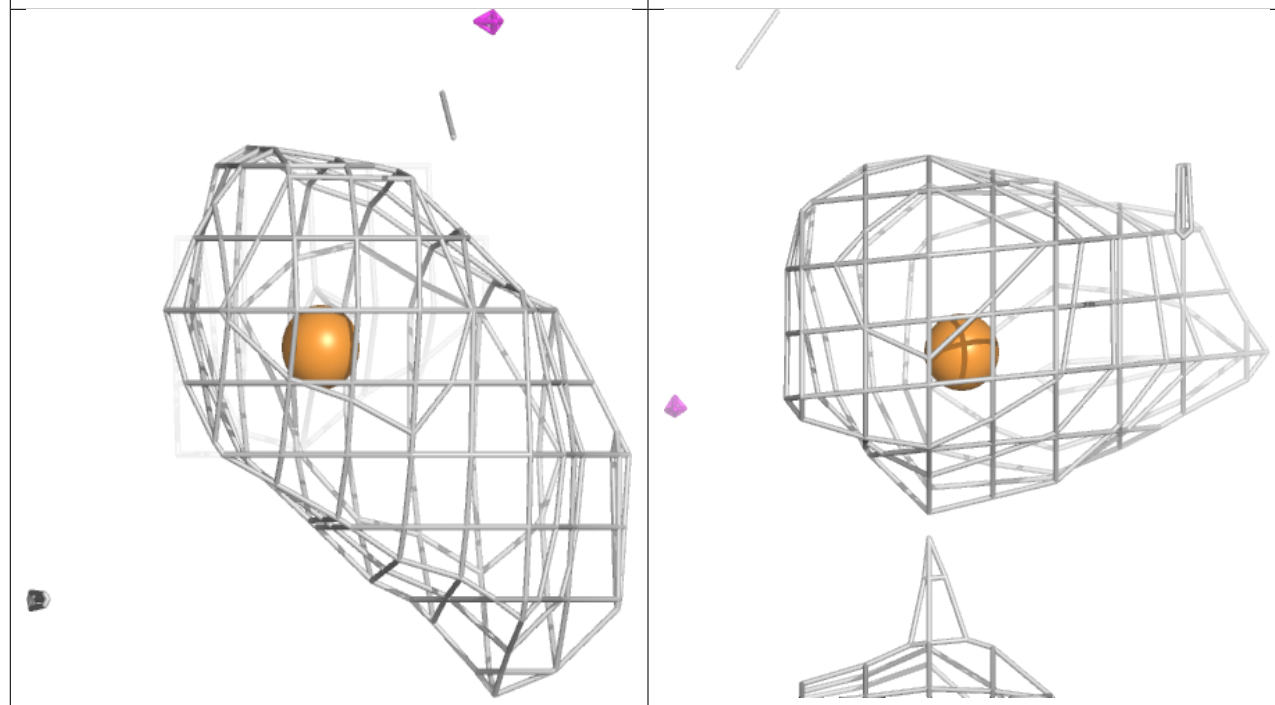
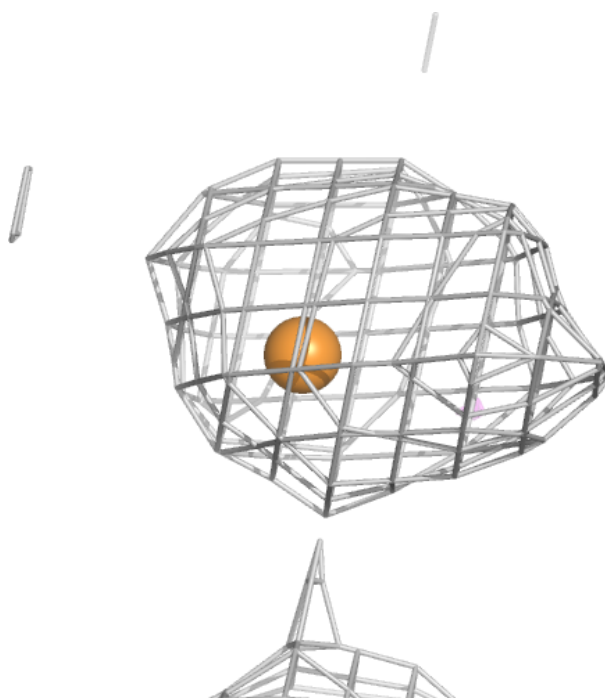
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	A	403	1/1	0.75	0.15	114,114,114,114	0
2	CU	K	401	1/1	0.75	0.26	136,136,136,136	0
3	GOL	A	404	6/6	0.76	0.17	58,66,69,70	0
3	GOL	A	405	6/6	0.81	0.22	60,71,78,80	0
3	GOL	A	407	6/6	0.82	0.18	48,59,63,66	0
2	CU	A	402	1/1	0.86	0.10	118,118,118,118	0
2	CU	A	401	1/1	0.86	0.23	122,122,122,122	0
3	GOL	A	406	6/6	0.88	0.13	35,39,40,40	0
2	CU	K	403	1/1	0.90	0.11	106,106,106,106	0
3	GOL	K	404	6/6	0.90	0.10	34,37,38,38	0
3	GOL	K	405	6/6	0.91	0.14	33,39,44,46	0
2	CU	K	402	1/1	0.95	0.05	75,75,75,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

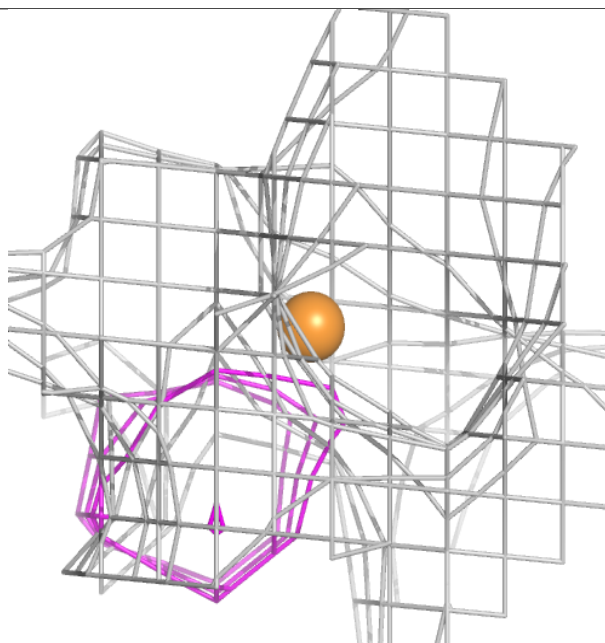
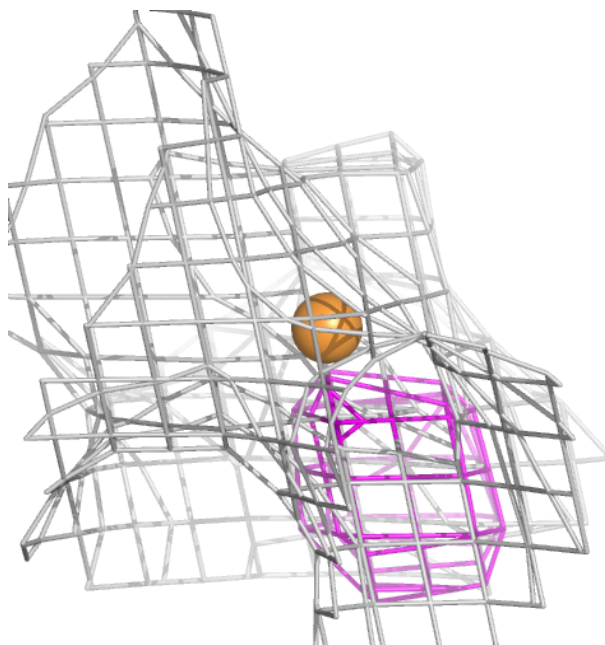
**Electron density around CU A 403:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



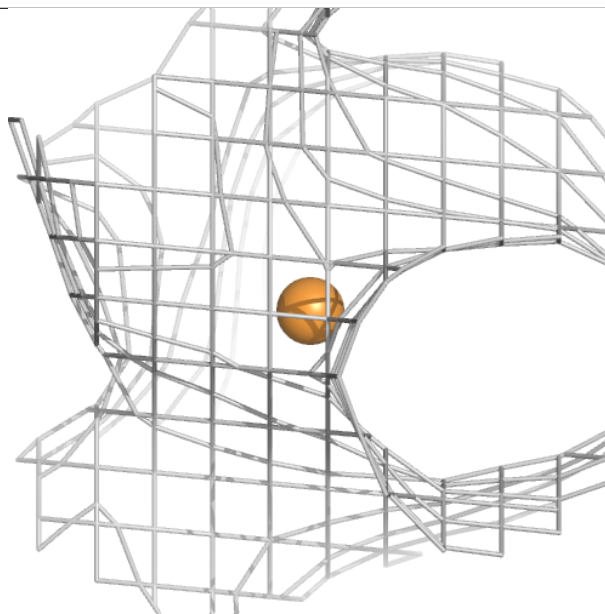
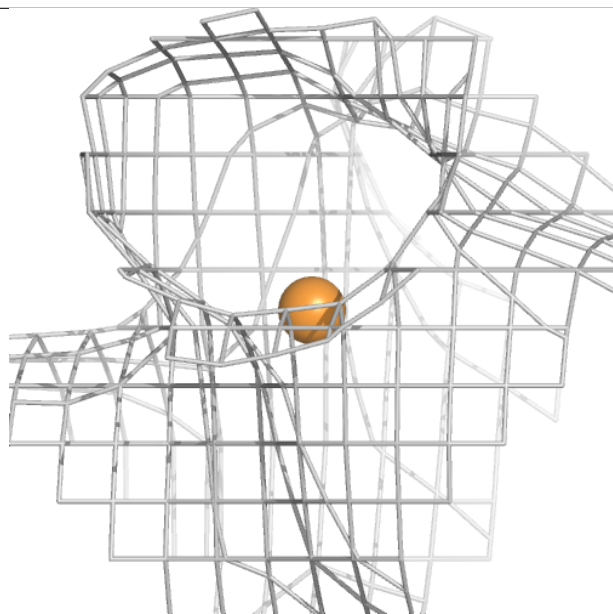
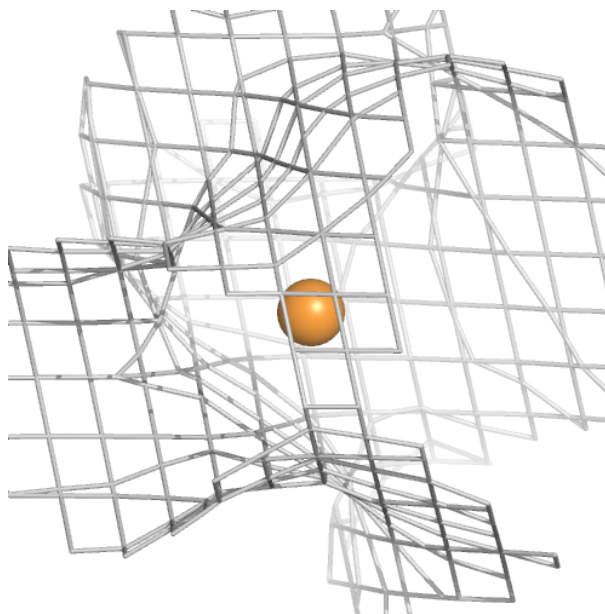
**Electron density around CU K 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



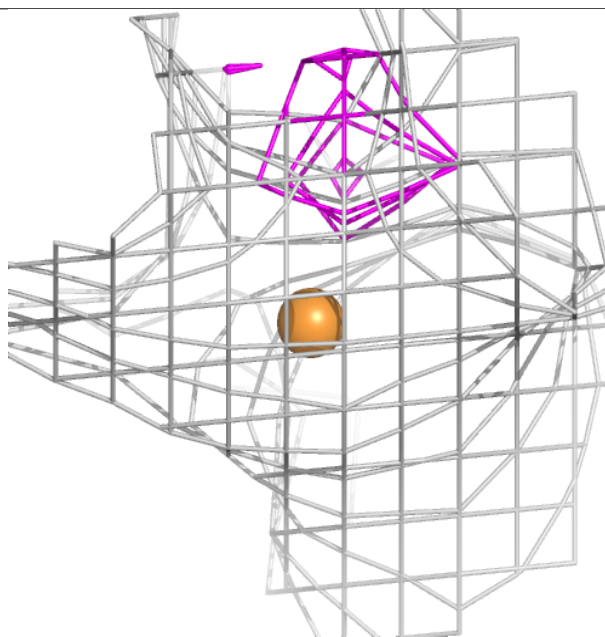
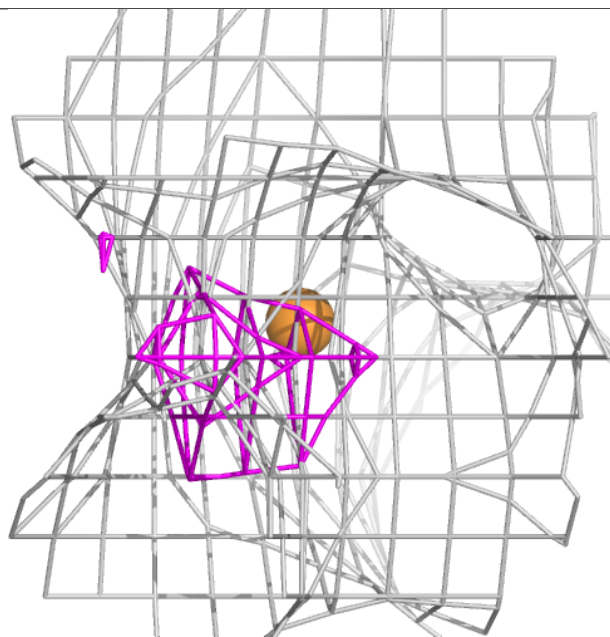
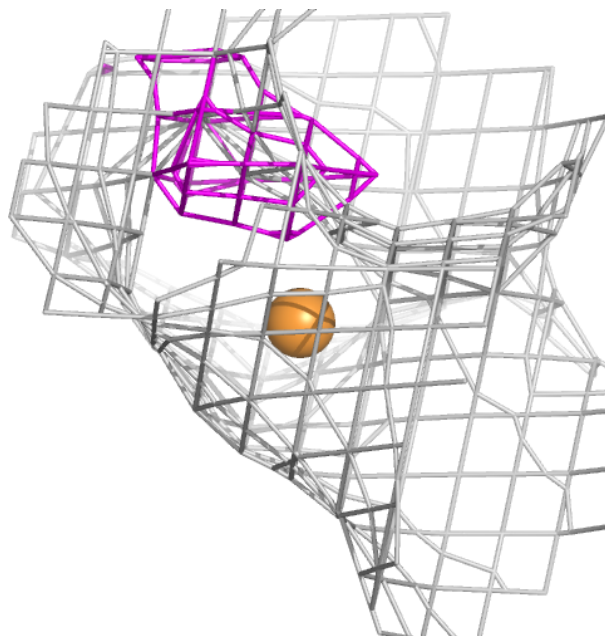
**Electron density around CU A 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CU A 401:**

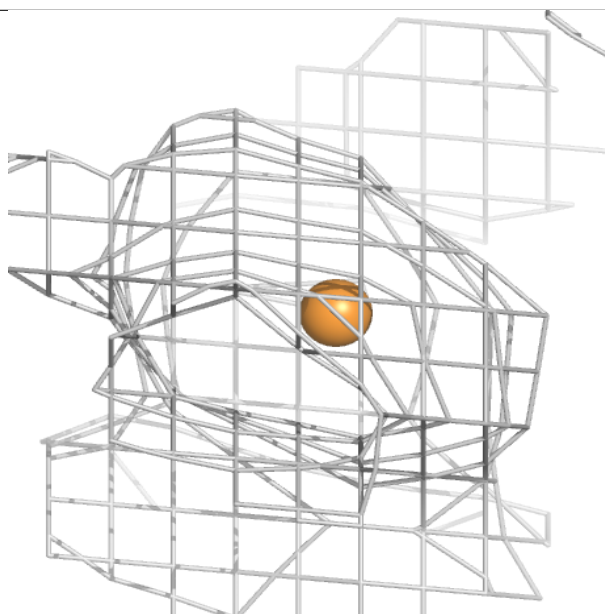
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CU K 403:**

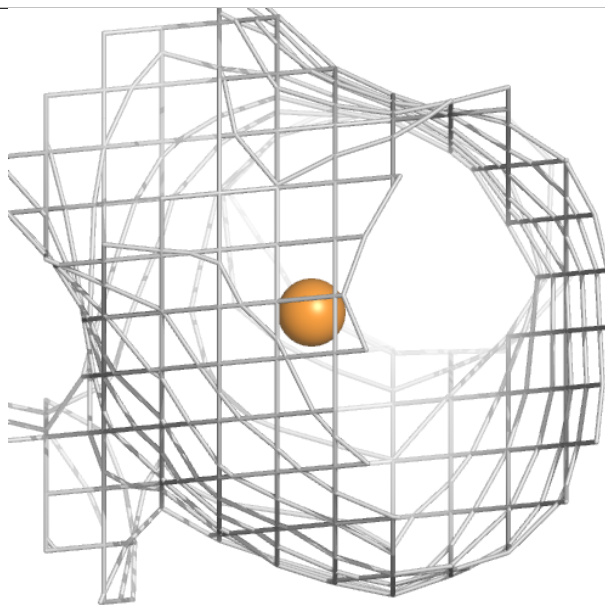
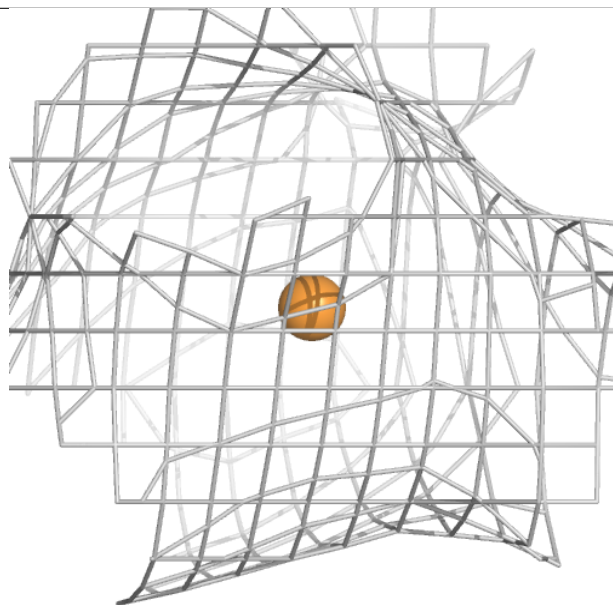
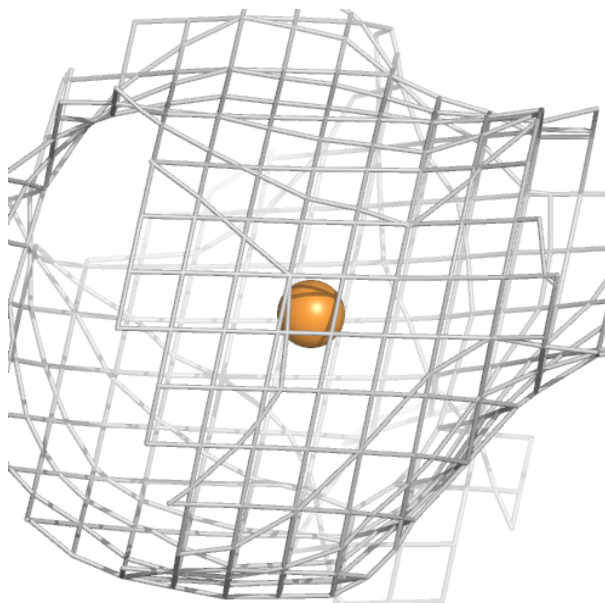
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CU K 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.